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This project attempted to systematically and quantitatively characterize the microstructure of heterogeneous materials and to use such information to predict rigorously the macroscopic behavior (e.g., effective moduli). By employing homogenization theory and the methods of statistical mechanics, we were able to mathematically describe the microstructure and, as a result, accurately determine the macroscopic response under a wide range of conditions. A goal was to treat seemingly disparate problems using a unified methodology. The generality of our approach enabled us to treat a wide class of two- and three-phase isotropic and anisotropic heterogeneous materials. This work will aid in leading to a highly cost-effective means of optimally designing heterogeneous materials for a particular application.

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Final Report

Microstructure and Macroscopic Behavior of Random Heterogeneous Materials

Grant No. F49620-92-J-0501

September 1, 1992 - February 28, 1996

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PREPARED FOR THE AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

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ABSTRACT

This project attempted to systematically and quantitatively characterize the microstructure of heterogeneous materials and to use such information to predict rigorously the macroscopic behavior (e.g., effective moduli). By employing homogenization theory and the methods of statistical mechanics, we were able to mathematically describe the microstructure and, as a result, accurately determine the macroscopic response under a wide range of conditions. A goal was to treat seemingly disparate problems using a unified methodology. The generality of our approach enabled us to treat a wide class of two- and three-phase isotropic and anisotropic heterogeneous materials. This work will aid in leading to a highly cost-effective means of *optimally designing* heterogeneous materials for a particular application.

I. GRANT ACCOMPLISHMENTS

In what follows we describe the accomplishments that we made on the AFOSR Grant No. F49620-92-J-0501. We published 11 refereed journal articles and gave 25 invited presentations on our AFOSR-related work.

1. Cross-Property Relations

An intriguing fundamental as well as practical question in the study of composite materials is the following: What can be said about various unknown effective properties when different properties of the composite are known? Such *cross-property relations* become especially useful if one property is more easily measured than another property. Since the effective properties of random media reflect important microstructural information about the medium, one might expect that one could extract useful information about one effective property given an exact determination of another property. Employing the so-called *translation method* (see Ref. 2 and references therein), we have derived the sharpest rigorous upper and lower bounds on the effective elastic moduli for two-dimensional, two-phase isotropic composites (i.e., transversely isotropic fiber-reinforced materials) in terms of the effective conductivity σ_e [2,6]. The former bounds are defined in the elastic moduli-conductivity planes by hyperbolas. Certain boundaries of these regions are realized by specific microgeometries and thus represent optimal bounds. We have also found the best available cross-property bounds for three-dimensional isotropic composites that link the effective bulk modulus κ_e to the effective conductivity σ_e [8].

How sharp are our cross-property estimates given an exact determination of one of the effective properties? To examine this question we use exact conductivity data and our cross-property relations to predict the effective bulk modulus κ_e for hexagonal arrays of superconducting, superrigid cylindrical fibers (phase 2) in a matrix. Our predictions are compared to exact bulk modulus data [1] (see Fig. 1). The agreement between our conductivity predictions and elastic moduli data is excellent (see Fig. 1). It is noteworthy

that *standard variational upper bounds* on the effective properties (such as Hashin-Shtrikman) here diverge to infinity as they do not incorporate information that the superrigid phase is in fact disconnected. In contrast, our cross-property upper bound uses the fact that the *infinite-contrast phase is disconnected via conductivity information.* In summary, cross-property relations provide a new and powerful way to extract important microstructural information on composites.

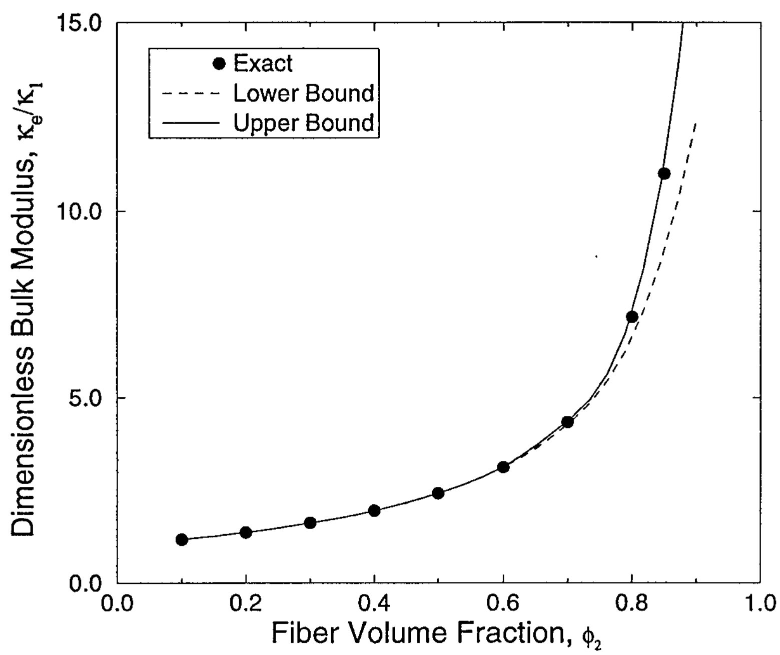

Figure 1: Comparison of the bulk modulus-conductivity bounds with the exact bulk modulus data (circles) [1] for a superrigid, superconducting hexagonal array of circular inclusions. Curves are the bounds using exact conductivity data.

More recently, we have applied the cross-property realtions to solid bodies that are damaged by cracks [7]. These are the first rigorous bounds on the effective moduli of cracked solids that do not require information about the crack density and geometry, quantities which are usually difficult to measure.

2. Imperfect Interfaces

The preponderance of theoretical predictions of the effective moduli of composites have been carried out assuming that the interface plays no role in determining the effective behavior of the materials, i.e., *perfect interfaces.* In real materials, interfacial effects can dramatically alter the effective behavior. For example, the Kapitza thermal resistance at the interface can be significant at sufficiently low temperatures, interfacial roughness can be appreciable enough to result in electrical resistance at the interface, and debonding at the interface can errode the effective elastic behavior of the composite.

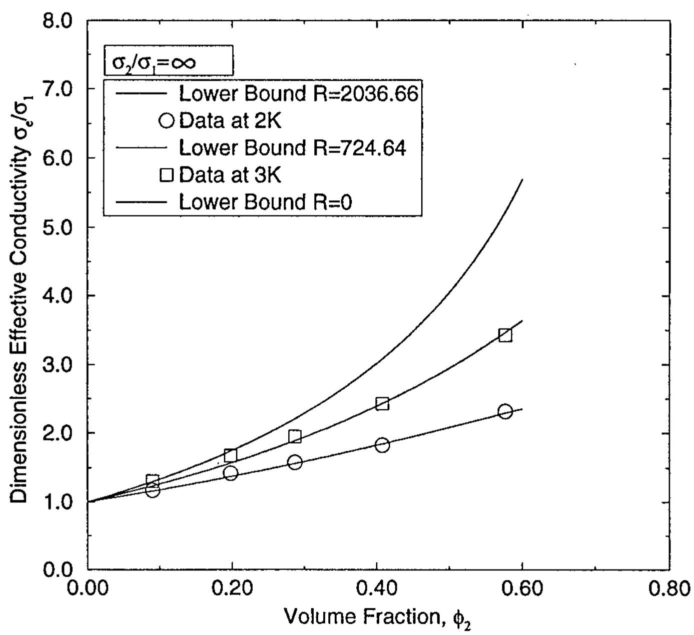

Figure 2: Comparison of the lower bounds of Torquato and Rintoul [5] on the dimensionless conductivity σ_e/σ_1 vs. inclusion volume fraction ϕ_2 to the experimental data (circles and squares) of De Araujo and Rosenberg for metallic particles in epoxy at 2 resistance values ($R = 0$ is perfect interface) corrsponding to two different temperatures.

We assert that in order to get sharp estimates of the effective properties of composites with imperfect interfaces, one must incorporate nontrivial morphological information about the interface. For example, previous elastic-moduli bounds for imperfect interfaces do not incorporate such nontrivial interfacial information and thus are not very sharp bounds. We begin by considering the problem of determining the effective conductivity σ_e of dispersions

of spheres with imperfect interfaces since: (i) it is mathematically easier than the elastic problem, and (ii) because (unlike the mechanical problem) experimental data exists for the interface property. For such a system we have developed rigorous bounds on σ_e [5] in terms of the conductivity of the inclusions, σ_2, conductivity of the matrix, σ_1, the dimensionless interface resistance, R, inclusion volume fraction ϕ_2, and higher-order morphological information, including interfacial statistics. Figure 2 shows that our new bounds give remarkably accurate predictions of the effective thermal conductivity of suspensions of metallic particles in epoxy matrices for two values of the Kapitza resistance R ($R = 0$ corresponds to a perfect interface).

We have recently evaluated the effective conductivity of periodic arrays of spheres with interfacial resistance [10]. Corresponding work was carried out for superconducting interfaces [11].

3. General Property Estimates

It is useful to obtain estimates of the effective mechanical properties that incorporate microstructural information beyond that contained in volume fractions alone. We have recently derived the best possible bounds on the effective elastic moduli of any transversely isotropic fiber-reinforced material (with a perfect interface) that depend upon three-point correlation function information [4]. We also found bounds on the effective bulk and shear moduli of suspensions of overlapping spheres [3].

We have also obtained the first nontrivial phase-interchange relations for the effective elastic moduli of both transversely isotropic and isotropic two-phase composites [9]. These relations are useful in studying such composite materials near their percolation thresholds.

4. Computer Simulations

Compared to theoretical studies, there has been much less research directed toward obtaining effective properties "exactly" from computer simulations, especially for *off-lattice or continuum models* (e.g., distribution of particles in a matrix). Such "computer experiments" could provide unambiguous tests on theories for well-defined model microstructures. We have applied the *boundary element method* to determine the effective elastic moduli of an idealized model of hexagonal arrays of infinitely long, aligned cylinders in a matrix (a model of a fiber-reinforced material) or a thin-plate composite consisting of hexagonal arrays of disks in a matrix [1]. This has led to the most comprehensive set of simulation data for the elastic moduli of this useful model system. We intend to apply this technique and related numerical methods (finite elements) to compute the effective moduli of random systems.

II. PUBLICATIONS

1. J. W. Eischen and S. Torquato, "Determining Elastic Behavior of Composites by the Boundary Element Method," **Journal of Applied Physics, 74**, 159 (1993).

2. L. V. Gibiansky and S. Torquato, "Link Between the Conductivity and Elastic Moduli of Composite Materials," **Physical Review Letters, 18**, 2927 (1993).

3. J. Quintanilla and S. Torquato, "New Bounds on the Elastic Moduli of Suspensions of Spheres," **Journal of Applied Physics, 77**, 4361 (1995).

4. L. V. Gibiansky and S. Torquato, "Geometrical Parameter Bounds on Effective Properties of Composites," **Journal of the Mechanics and Physics of Solids, 43**, 1587 (1995).

5. S. Torquato and M. D. Rintoul, "Effect of the Interface on the Properties of Composite Media," **Physical Review Letters, 75**, 4067 (1995).

6. L. V. Gibiansky and S. Torquato, "Rigorous Link Between the Conductivity and Elastic Moduli of Fiber-Reinforced Composite Materials," **Philosophical Transactions of**

the Royal Society of London, 343, 243 (1995).

7. L. V. Gibiansky and S. Torquato, "Bounds on the Effective Moduli of Cracked Materials," **Journal of the Mechanics and Physics of Solids, 44**, 233 (1996).

8. L. V. Gibiansky and S. Torquato, "Connection Between the Conductivity and Elastic Moduli of Isotropic Composite Materials," **Proceedings of the Royal Society of London A, 452**, 253 (1996).

9. L. V. Gibiansky and S. Torquato, "Phase-Interchange Relations for the Elastic Moduli of Two-Phase Composites," **International Journal of Engineering Science, 34**, 739 (1996).

10. H. Cheng and S. Torquato, "Effective Conductivity of Periodic Arrays of Spheres with Interfacial Resistance, **Proceedings of the Royal Society of London A**, in press.

11. H. Cheng and S. Torquato, "Effective Conductivity of Suspensions with a Superconducting Interface," **Proceedings of the Royal Society of London A**, in press.

III. INVITED TALKS AND CONFERENCE PRESENTATIONS

1. **Connection Between Morphology and Effective Properties of Heterogenous Materials**, American Society of Mechanical Engineers, Anaheim, California, November, 1992.

2. **Heterogeneous Materials**, Seminar given at the University of Pennsylvania, Philadelphia, Pennsylvania, November, 1992.

3. **Morphology and Macroscopic Behavior of Random Heterogeneous Media** Seminar given at Rutgers University, New Brunswick, New Jersey, December, 1992.

4. **Heterogeneous Materials: Macroscopic Properties and Microstructure**, Exxon Research, Annandale, New Jersey, January, 1993.

5. **Heterogeneous Materials for Fun and Profit**, Seminar given at the University of Pennsylvania, Philadelphia, Pennsylvania, March, 1993.

6. **Heterogeneous Materials: Macroscopic Behavior and Microstructure**, Seminar given at Michigan State University, East Lansing, Michigan, April, 1993.

7. **Micostructure and Macroscopic Behavior of Heterogeneous Media: A Unified Approach**, 69th Statistical Mechanics Meeting, Rutgers University, New Brunswick, New Jersey, May, 1993.

8. **Rigorous Link Between the Effective Elastic Moduli and Effective Conductivity of Composite Materials**, MEET'N'93 (Joint ASME, SES, and ASCE Meeting), Charlottesville, Virginia, June, 1993 (with L. V. Gibiansky).

9. **Macroscopic Behavior of Random Media from the Microstructure**, MEET'N'93 (Joint ASME, SES, and ASCE Meeting), Charlottesville, Virginia, June, 1993

10. **Numerical Simulations of the Mechanical Properties of Multi-phase Composites**, MEET'N'93 (Joint ASME, SES, and ASCE Meeting), Charlottesville, Virginia, June, 1993 (with E. J. Garboczi and A. R. Day).

11. **Macroscopic Behavior of Random Heterogeneous Materials from the Microstructure**, National Science Foundation Workshop on *Statistical Characterization of Material Microstructure and its Relation to Material Performance*, The Catholic University of America, Washington, DC , June, 1993.

12. **Unified Methodology to Quantify the Morphology and Properties of Inhomogeneous Media**, Electrical Transport and Optical Properties of Inhomogeneous Media Conference, Guanajuato, Mexico, August, 1993.

13. **Unified Methodology to Characterize the Microstructure and Properties of Heterogeneous Materials**, Institute for Advanced Study, Princeton, New Jersey, October, 1993.

14. **Unified Methodology to Quantify the Morphology and Properties of Heterogeneous Materials**, Worcester Polytechnic Institute, Worcester, Massachusetts, October, 1993.

15. **Link Bewteen the Conductivity and Elastic Moduli of Heterogeneous Materials**, American Institute of Chemical Engineers, St. Louis, Missouri, November, 1993.

16. **New Cross Property Relations for Composites**, American Society of Mechanical Engineers, New Orleans, Louisiana, December, 1993.

17. **Rigorous Link Between the Microstructure and Bulk Properties of Heterogeneous Materials**, Materials Research Society Meeting, San Francisco, California, April, 1994.

18. **Macroscopic Behavior of Random Media from the Microstructure**, Society of Industrial and Applied Mathematics on *Emerging Issues in Mathematics and Computation from the Materials Sciences*, Pittsburgh, Pennsylvania, April, 1994.

19. **Unified Methodology to Characterize the Microstructure and Properties of Composite Media**, Society of Industrial and Applied Mathematics on *Emerging Issues in Mathematics and Computation from the Materials Sciences*, Pittsburgh, Pennsylvania, April, 1994.

20. **Microstructure-Property Relations for Composite Materials**, Gordon Research Conference on *Solid State Studies in Ceramics*, New Hampton School, New Hampshire, August, 1994.

21. **Unified Methodology to Quantify the Microstructure and Properties of Composite Materials**, International Union of Theoretical and Applied Mechanics Syposium on *Microstructure-Property Interactions in Composite Materials*, Aalborg, Denmark, August, 1994.

22. **Structure and Properties of Disordered Heterogeneous Media** *Controlling Complex Microstructures*, American Ceramics Society, New Orleans, Louisiana, November, 1995.

23. **Rigorous Link Bewteen the Electrical and Mechanical Properties of Composite Materials**, Symposium on Electrically Based Microstructural Characterization, Materials Research Society, Boston, Massachusetts, November, 1995.

24. **Random Heterogeneous Materials: Structure and Properties**, Seminar given at SUNY Stony Brook, Stony Brook, New York, February, 1996.

25. **A Unified Approach to Quantify the Structure and Properties of Heterogeneous Materials**, Seminar given in the Ceramics Dept. at Rutgers University, New Brunswick, New Jersey, February, 1996.

IV. PERSONNEL

In addition to the principal investigator, Prof. Salvatore Torquato, the salaried research group at Princeton University consisted of two postdoctoral associates, Dr. Leonid Gibiansky and Dr. Hongwei Cheng, and a graduate student, John Quintanilla, who will complete his Ph.D. degree at the end of the year.